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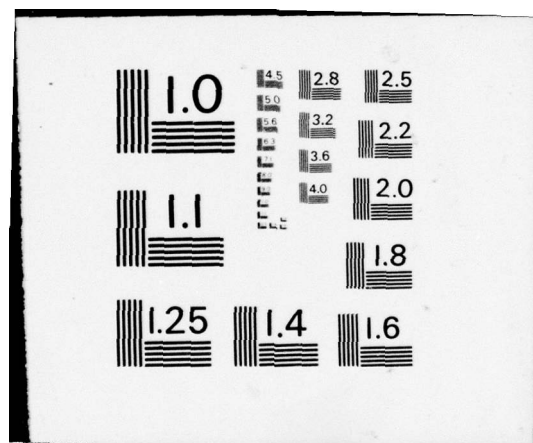
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Theory of Solid Surfaces

J.C. INKSON and P.W. ANDERSON

Cavendish Laboratory,

Cambridge, CB3 0HE.

1st May, 1976.

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Abstract

The purpose of this report is to describe the work performed in the Theory of Condensed Matter Group of the Cavendish Laboratory during the period 1973 - 1975, with A.F.O.S.R. support. A wide range of work is described on surface and bulk properties of materials as well as the application of solid state techniques to the theory of nuclei and neutron stars. On surfaces an important new development is described in the theory of catalysis which relates it to the multiple-valency states of transition metal atoms in semiconductors. Work upon metal semiconductor interfaces and its application to Schottky barriers and photoemission is described. Related to this is the continuing investigation into surface induced superconductivity and reasons are suggested as to why the goal may be illusionary. The developments of the calculation of the optical scattering potential for surface scattering (as in LEED) are described and its gross properties explained in terms of a simple model.

The application of local methods to semiconductors is becoming more and more important and should be applied to a large range of surface problems in the next few years. Two developments are described here, on bulk properties, the calculation of the dielectric response, and the application of the Anderson chemical pseudopotential to a range of bulk properties of semiconductors and 'non-simple' materials. This last method shows promise of connecting solid state physics to the more chemical ideas of bond properties. Also using a local method we describe some promising work on the Laves phases of transition metal alloys which are too complicated to calculate in the normal k -space form but have important technical applications. Finally in solids we describe the recent work on spin glasses which breaks new ground in the understanding of this system and has important consequences for the theory of a number of polymer related problems.

We conclude with a miscellany of the application of solid state techniques to unusual problems namely neutron stars and nuclei.

In the appendix to this report will be found a review of the state of the art in Europe in important areas of surface science.

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1. Introduction

This report is a survey of the various work supported during the period 1973-1975 by the USAF Theory of Solid Surfaces grant (73-2449 A). In many cases the support has only been a very small proportion of the total so we have had to limit to some extent the report since only a full statement of all the work done by the Theory of Condensed Matter (T.C.M.) group would cover the effective area of support which this grant has provided. With this provision in mind this report can be divided into the two basic areas of surface and bulk studies but has in addition sections on neutron stars and nuclei where existing solid state techniques have been applied to these unusual areas. The personnel involved have changed considerably over the three years involved and of the workers represented in this document only Dr. Inkson remains at the Cavendish. This has a direct bearing upon the report since in many cases the description of some of the work is shorter than we would wish as the original author is unavailable. For further reference we have provided a full bibliography of not only the work directly supported by the U.S.A.F. but also the full list of papers published by T.C.M. during the same period. Also added as an appendix is a review of the state of the art in European Surface Science.

One major piece of work which is not included here is the book written by Professor Anderson during his period. This contains a number of original ideas and occupied a fair proportion of his time. He continued however to interact strongly with T.C.M. especially through his students.

2. Surfaces

2.1 Catalysis

With Mr. Haldane, Professor Anderson has developed his ideas of the telescoping of the valence states of transition metal atoms when associated with various substrates, in particular the heme ring in biological systems and the semiconductor surface (ref. 1). The importance of this work cannot be overestimated since it is basic to an understanding of catalysis.

Fundamental studies of the phenomenon of catalysis seem to agree only on its extreme complexity. Any or all of a number of phenomena may play an important role: e.g. geometric surface properties, special reaction pathways, even complicated many-body fluctuations of the

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electronic structure of the substrate.

In spite of that there seem empirically to be certain generalities about catalysts, or even more generally about systems which act as reaction substrates, such as enzymes. Some of these are as follows:

- (1) Neither good metals nor good insulators serve well.
- (2) Transition metals, especially from the higher end of the series, are most reliable - platinum playing the role of the universal electrochemical catalyst.
- (3) There is a clear correlation with magnetism.
- (4) The phenomenon of mixed valences often plays a role of some sort.

A case in which several of these hints as to the nature of the process seem to be in operation is that of the role of the heme ring in biological reactions. It is striking that evolution has managed to insert ring "metallic" groups - the heme ring, especially - into many enzymes, as well as, often, transition metal atoms. It seems clear that having stumbled on the heme ring, evolution needed to look no further and inserted it into many reaction pathways - what does it do?

Empirically, it is clear, at least in the case of hemoglobin, that the effect of the heme is, for some unknown reason, to bring four usually incompatible states of the iron ion remarkably close to each other in energy: The low- and high-spin, ferric and ferrous states, all of which are stable given slight modifications of ligands, pH, etc.

This case reminds one of yet another case of accelerated reaction rates and mixed valences, which in a sense may be the simplest of all catalysed reactions: recombination of electrons and holes in semiconductors. This is highly accelerated when transition metal impurities are present, such as Au, Cu, or Mn. From paramagnetic resonance measurements, it is known that each of these can be found in several distinct valence states which are separated by energies less than the ~ 1 eV gap. It is the availability of this multiplicity of states of different nominal charge over the relevant range on energy which seems to be vital to the recombination reaction.

An ability therefore to "telescope" the valence states of adsorbed atoms would be of very great value to a catalyst, for two reasons:

- (1) It would increase reaction rates by making available different valence states of the reactants. For instance, if one could remove the $H + H \rightarrow H^- + H^+$ energy difference so that all species are present in equilibrium, undoubtedly many reactions would be accelerated.
- (2) This would make the substrate less liable to poisoning or to removal reactions, since strongly-bound states of adatoms would

easily be superseded by others - e.g. if the energies of $2H$ and H_2 are similar, H 's can easily recombine and drift away leaving the surface unpoisoned.

Thus while they have no direct experimental evidence at all to back up the suggestion, they have suggested that useful catalysts (or reaction substrates such as enzymes) should have this property of telescoping the valence states of adatoms. They find that this requires a feature of the electronic structure which actually is present in metallic catalysts: one or more step features in the density of states. Thus it may be that in analyzing the multiple-valency states of transition metal atoms in semiconductors or in heme rings, they may well be discussing a phenomenon of much more general importance.

2.2 Metal Semiconductor Interfaces

Schottky Barriers form an area of major technological interest since the formation of a potential barrier between a metal and a semiconductor alters the conduction properties of the system in either a beneficial, if one needs a rectifier, or detrimental form if one is interested in ohmic contact. The physics of the barrier is however not well understood even though it is nearly forty years since the gross properties were recognised. In our work (ref. 2,3,4) we have considered a completely different approach to the usual one electron, surface state type of model (e.g. Mead in Solid State Electronics, 1966, 9, 1023) that is one in which the changes in the exchange and correlation energy in the semiconductor are calculated near the metal. This results in a reduction of the band gap of the semiconductor leading to a simple picture of the barrier formation and in particular its dependence upon the 'ionicity' of the semiconductor (ref. 4).

In summarising our work in this area it is better to go non-chronologically. In a semiconductor the exchange and correlation energy for the valence and conduction bands are different because the effective interaction changes across the gap (ref. 5,6). This results in a 'many body' contribution to the band gap which is approximately a constant fraction of the direct gap but can be as large if not larger than the indirect gap (ref. 5). If the electron-electron interaction can be changed in some way then one would expect the semiconductor band gap to show a corresponding change. This is precisely what happens when one puts a metal on top of a semiconductor. Near the metal large

changes occur on the semiconductor which result in a narrowing of the effective band gap. In the case of covalent semiconductors this can amount to all of the indirect band gap of the semiconductor so that it becomes metallic at the surface and so screens the rest of the semiconductor from the metal. This would result in a Schottky barrier independent of the overlying metal as observed in practice. In the case of an ionic semiconductor the effect is not as drastic the gap is only reduced slightly at the surface so that the Schottky barrier should still be determined primarily by the metal. Again this is just what is seen so that this model is at least as successful in describing the major effects as the "surface state" theories. An important byproduct of this work is the investigation of the interaction near the interface and the calculation of the collective oscillations (or plasmons) localised in that region (ref. 3). This has enabled us to treat much more realistically a number of problems associated with metal semiconductor interfaces and free surfaces as we describe in the following sections.

At present Mr. N. Swingler is working with me on extending the Schottky Barrier work to the calculation of the charge densities in the region of the interface. This is a very difficult problem if one is to have any real physical insight rather than the sledgehammer technique of the large scale numerical calculations which have been performed (and still do not seem to give an answer to the problem).

On other project which has had very indirect support is the study of infrared photoemission from negative electron affinity photocathodes produced by a layer of Caesium oxide on Gallium Arsenide. We have studied the effect of the Gallium Arsenide substrate on the efficiency of the photoemission. We have achieved a number of substantial results, (refs. 7,8,9,10,11) the most spectacular being the proof that the large-difference between the efficiency of the activated 111 A and 111 B faces is due to the intrinsic properties of Gallium Arsenide and not as a result of a better activation (ref. 9). This should save a substantial amount of unnecessary experimental work.

2.3 Superconductivity at Surfaces

There has been continued speculation that surface induced superconductivity by way of a boson exchange other than a phonon could offer the possibility of higher critical temperatures than the 'normal'

form. During the course of this grant we have considered the two major possibilities at a metal semiconductor interface, that is superconductivity by way of the exchange of excitons (ref.12) and interfacial plasmons (ref.13). In both cases we have found an adverse effect and our work has led us to believe that there is a fundamental flaw in the previous and current speculations on this subject.

Work by Allander Bray and Bardeen (Phys. Rev.B7, 1973,1020) suggested that high temperature superconductivity could be achieved in metal semiconductor junctions because of the attractive nature of the exciton exchange process in the neighbourhood of the interface. The work contained however a number of anomalies in particular it suggested that as the semiconductor became more metal like the effect became stronger. Taking this as our starting point we investigated in more detail the process of exciton exchange at the interface (ref.12). We found that the exciton process was just another manifestation of the normal screening process which occurred in the metal by way of the exchange of electron hole pairs. This very attractive process is the one which reduces the bare interaction to the screened one in normal metals. When one introduces an interface into the problem two things happen the new exciton exchange is introduced on the semiconductor side but the old metal electron-hole exchange is removed so that it is the difference between these two which is the important factor. In previous treatments the exciton exchange had been added on top of the electron-hole process. Since exciton exchange in a semiconductor is less effective than electron hole exchange in a metal the net result when one considered the process in detail is such as to reduce the superconducting critical temperature in the metal. To investigate whether this compensation was typical of interfaces we considered the obvious alternative mechanism which is the exchange of interfacial plasmons, the new collective modes which we introduced at the metal semiconductor junction (refs.3,13).

This is particularly interesting because firstly the electrons interact very strongly with plasmons in contrast to the excitons so any effect could be large. Secondly the sensitivity of the interface plasmons to the separate components would make it a very flexible system on which there is already a high technological expertise. We found that there was again a negative effect when considering the metal but it could send the semiconductor superconducting when it was a border-line material as say lead telluride or marginally aid the

superconductivity in a system like tin telluride. The most interesting point about this was that the reasons for the failure of this mechanism to give high temperature superconducting were exactly the same as in the previous situation. We feel that when one does calculations of this type it is very important to consider the system as a whole paying particular attention to the basic sum rules. Continuing this work and extending it to the layered compounds (i.e. a multi surface system), I (J.C.I.) have a research student. Although this will not lead to any high temperature superconductor the transport properties will certainly be substantially modified in these systems by the low lying collective modes. I would like to mention in passing that of course if the air force took calculations like Professor Anderson's or mine ^{seriously} on these systems they could save a considerable amount of money in the fruitless search for these exotic superconductors.

2.3 Free Surfaces

In going from a vacuum into a metal an electron moves into a region of high electron density where correlation and exchange effects play a large part in determining the energy and lifetime of the state. Deep inside the metal where surface effects are negligible we already have a fair description of the effect upon the electron states in terms of the exchange and correlation potential as calculated in a number of standard approximations . The potential is in general complex; the real part corresponds to the normal correlation and exchange potential which must be added to crystal potential for the calculation of the band structure while the imaginary part is a measure of the lifetime of the state concerned. In the calculation of the effects of the electron interaction with the metal surface, (ref.14) both parts of the potential are of course very important and together they form a complex optical potential for scattering, akin to the potential used in nuclear physics. In order to be useful this potential should include two things, firstly the variation with position and secondly the variation of the two components with the state considered. Consider for instance the formulation of the many body problem which describes the potential as arising from the excitation of plasmons; virtual excitation gives rise to the real part while real excitation is the decay process responsible for the imaginary part and hence finite lifetime of the state. How does the introduction of a surface effect the potential?

It is known that the image potential asymptote of the real part of the potential can be considered as a consequence of the virtual excitation of the surface plasmons which effectively screens out the electron field from the bulk metal. Provided the electron has an energy higher than the surface plasmon energy there is also the possibility of real surface plasmon excitation and hence the potential will be complex inside the metal even before bulk plasmon processes become available for decay. Well away from the surface on either side these processes will become frozen out because of the fall off of the electron-plasmon coulomb interaction. The real part of the potential is known to be relatively insensitive to the energy of the state. For an electron of fairly high energy (i.e. both bulk and surface processes easily available), as it moves from the bulk metal towards the surface the bulk plasmon contribution to the potential will start to fall off as the interaction changes but at the same time surface plasmon processes start to increase in importance thus, on the metal side, we would expect some form of compensation between these two processes. This is very effective for the real part of the potential, where of course there is no restriction on the excitations available, but not so much for the imaginary part especially at the low energies. This is again related to the effect mentioned in the previous section.

The actual calculation of this complex potential (ref 14) requires large numerical computing but the gross features do not differ very much from those expected in the above discussion. It is now being used in the LEED calculations in an attempt to improve agreement with experiment.

2.4 Surface Reconstructions

When a uniform semiconductor crystal is cleaved and then the resulting surface studied it is very commonly found that extra periodicities have appeared upon the surface which are related to the projection of the original lattice. These superlattices have been the subject of a number of investigations and many reasons put forward to explain the particular patterns which are seen. In the recent work of Anderson and Tosatti (refs.15,16) however we believe a major advance has been made. This new approach rests upon two observations, firstly the surface dangling bonds form a two dimensional metallic system

which can be considered apart from the rest of the crystal and secondly this system is inherently unstable against the formation of charge density or spin density waves. The instability can best be seen by considering the fermi surface of this two dimensional metal; it is approximately hexagonal so that a phonon of a single wavevector will couple together a large part of the fermi surface (i.e. almost a third). This results in a softening of the phonon to the extent where its energy goes to zero and the system reconstructs accordingly. In the same way electron hole pairs can couple in the surface and form an excitonic induced metal insulator transition leading to spin density waves and a magnetically ordered system which would be observable through polarised LEED. The periodicities of many of the higher order reconstructions seen on silicon and germanium (111) surfaces agree with those expected in the charge density wave case. This work is very closely connected of course to the work on Peierls transitions and the reconstructions in layer materials which are at present being investigated in this laboratory by Dr. Yoffe and his colleagues.

3. Bulk Studies

3.1 Physics of Semiconductors

One aspect of semiconductors and indeed to a lesser extent most materials is the nonuniformity of the charge density which, for phonon spectra or many body effects such as collective excitons, can produce large effects. These are incorporated in the dielectric response of the system in the form of off-diagonal elements (i.e. the dielectric function becomes a matrix). If we are to treat the surface effects such as phonons in such a system then we have to have a fairly reliable method of calculating the matrix.

We have made two calculations of this, the first (ref. 17) was from a fairly standard pseudopotential basis with which we were familiar and could be certain of the approximations introduced. This calculation produced a number of new results the most important of which was the connection of the strength off diagonal elements to the topology of the Jones zone (the extended zone which includes all of the valence electrons). This enabled us to discuss the behaviour of the matrix as the system was altered to go through the whole ionic-covalent-metallic series. This has useful consequences for evaluating phonon and optical calculations as well as giving estimates of the importance

of the local field effects as in the superconductivity discussion (section 2.3). The main difficulty with this type of calculation however is that it is not the most useful if one has a surface or other discontinuity present; in this case a local form is much more natural. This we are at present developing and extending based upon a Wannier function representation similar to that used by Hanke and Sham (Phys. Rev. Lett (1974) 33, 582). Although at present we are clearing up difficulties associated with the optical spectra of diamond and silicon we eventually hope to apply it to surface phonon studies and the problem of surface reconstruction associated with semiconductor surfaces (ref. 15,16,18). The work on the effect of the electron-electron interaction on the semiconductor band gap (ref. 6) is summarised in the Schottky barrier section.

Connected with the move towards more local (i.e. allied to tight binding) approaches to semiconductor problems has been the work of Bullett (refs. 19-26) in our group which is based upon the work of Anderson on the chemical pseudopotential (U.S.A.F. F61052-68-C-0049). It is an experimental fact that many bonds have very nearly constant properties. The equilibrium distance between two atoms A and B connected by a fixed type (single, double, etc) of covalent bond varies little between different molecules and crystals. Other typical bond properties such as force constants, dipole moment, polarizability etc are discussed in many textbooks of physical chemistry. It is chiefly because of this transferability of so many bond properties that the concept of the chemical bond is so valuable. The work is concerned with a localized orbital description of covalency in the framework of Anderson's chemical pseudopotential theory (refs. 19-26).

At first sight these characteristic bond properties present a problem, for we know that electrons in molecules are not localized. Quantum mechanics requires that the eigenfunctions, even in a one-electron approximation, extend over the entire system. The original formulation of molecular orbital theory followed the intuitive idea that individual electrons move more or less independently in the average field of all the other electrons in the system; molecular orbitals were extended and not suited to a description of the localized bond properties of a polyatomic system. However, it was pointed out by Fock that when we write the wavefunction as a Slater determinant of molecular orbitals, we could equally well use a determinant of localized orbitals, which are linear combinations of the occupied molecular orbitals.

Anderson used pseudopotential ideas (contract F61052-68-C-0049) to develop a simpler theory which is particularly suited to explaining some of the semi-empirical ideas of chemistry. Indeed, Anderson was able to show how the Hückel parametrization scheme for conjugated systems follows directly from his chemical pseudopotential equations and that the appropriate local orbitals for Hückel theory can easily be calculated and are almost identical to the simple atomic orbitals.

Bullett has applied Anderson's theory to a large number of situations. The band energies for Carbon and Silicon have been calculated along with such measurables as the bond lengths and bulk moduli (refs. 19, 20). The power of this method is illustrated by the application to the layer and chain elements As, Se, Sb, Te where a similar calculation was performed (ref.24) and achieved good agreement with those calculated by other more conventional methods. The local methods as we have mentioned are particularly suited to some surface calculations and connect well with the chemists ideas of "dangling bonds". Bullett (ref.25) has applied his method to the (111) surface of silicon and carbon (in a diamond lattice) to calculate the relaxed position of the unreconstructed surface. He found that the separation of the outermost layers decreased to about 40 % of its bulk value while the surface energy was found to be 1.0 eV for silicon and 1.6 eV for carbon.

Finally, another aspect of semiconductor work which could have important technological aspects is the reduction of the band gap of semiconductors as the doping of the crystal is increased. I have been looking at this (ref.6) in the last few months and found that the decrease is marked and is larger than most previous calculations would have predicted due to the inclusion of another contribution which had been neglected before. This is in fact another application of the general many body approach we are developing towards real systems and materials as against the electron gas which has been the centre of interest up to now.

3.2 Spin Glasses

A new theory (ref.28) of the class of dilute magnetic alloys, called the spin glasses, is proposed which offers a simple explanation of the cusp found experimentally in the susceptibility. The argument is that because the interaction between the spins dissolved in the matrix oscillates in sign according to distance, there will be no mean

ferro- or antiferromagnetism, but there will be a ground state with the spins aligned in definite directions, even if these directions appear to be at random. At the critical temperature, the existence of these preferred directions affects the orientation of the spins, leading to a cusp in the susceptibility. This cusp is smoothed by an external field. If the potential between spins on sites, i, j is $J_{ij} s_i \cdot s_j$ then it is shown that

$$kT_c = \left(\sum_{ij} \frac{2J_{ij}^2}{9} \epsilon_{ij} \right)^{\frac{1}{2}}$$

where ϵ_{ij} is unity or zero according to whether sites i and j are occupied. Although the behaviour at low T needs a quantum mechanical treatment, it is interesting to complete the classical calculations down to $T = 0$. Classically the susceptibility tends to a constant value at $T \rightarrow 0$, and the specific heat to a constant value.

3.3 Laves Phases in transition metal alloys (ref.29-31)

The celebrated Hume-Rothery type rules, associating alloy phase stability with average electron concentration, are not yet understood theoretically in transition metal alloys. Two major questions arise. Firstly, what features are necessary to produce a correlation of the stability of phases with ranges of electron-to-atom ratio e/a ? Secondly, why is average e/a a sufficient parameter, i.e. why can we use a common band model, in which we neglect differences in the self-energies of the alloy components?

The Laves phases are a set of three related complex structures which occur frequently in AB_2 binary alloys, and are isomorphs of $MgCu_2$, $MgZn_2$ and $MgNi_2$. Transition metal alloys exhibit regular structural trends between the three Laves phases with varying composition. This has attracted a substantial amount of experimental and theoretical work, but until now no first-principles calculation of electronic energy has been possible. We have computed d-band densities of states by the recursion method of Haydock, Heine and Kelly, the more conventional method via the band structure $E(k)$ being impractical due to the large number of atoms per cell. We thus make the usual assumption of transition metals, that the structural variation of d-electron binding dominates that of the sp-band. The calculation is properly termed a common-band model since it is better than the rigid-band and virtual

crystal approximations. Gaussian quadrature was used to calculate integrated quantities such as the number of d-electrons per atom, e/a , and their total energy per atom, U , for a given Fermi level E_F . Of course the total energy should include various electrostatic, exchange, and correlation terms beside the sum of one-electron energies, but these are expected to be nearly identical for the three structures which for ideal c/a ratios have identical interatomic distances and densities, only differing in stacking sequence.

The energy differences per formula unit are of the order of one millirydberg, but the absolute value should only be taken as an approximate lower bound for real alloys, because of the parameters used. In the region where alloys lie, about $e/a = 3$ to , we find that the most stable structures are firstly $MgCu_2$ (from $e/a = 3.4$) then $MgZn_2$ (from $e/a = 4.9$), next $MgNi_2$ (around $e/a = 6.5$ up to 6.9), again $MgCu_2$, and firstly from $e/a = 7.7$, $MgNi_2$. A notable feature is the cyclic variation, giving regions of stability associated with ranges of e/a .

Of the 76 transition metal alloys forming Laves phases, the structures of 60 are correctly accounted for by the theory without any adjustment. This result has been achieved without varying any optimising parameters, and so indicates the general correctness of the model within the approximations of the theory.

We may conclude that the d-band binding in a common band model is the major influence determining which of the three Laves phases is stable in a given alloy, contrary to some suggestions of other authors. We may semi-empirically incorporate the major factor neglected so far, the site diagonal energy differences. For simplicity we work in terms of group number difference, G , between the group numbers in the periodic table of the B and A-site elements (averaged over A and over B-sites for pseudobinaries). Those alloys for which the uncorrected theory fails, have a high average G , and inclusion of G in the theory gives phase boundaries that curve downwards from the theoretical values at $G = 0$ in agreement with experiment.

4. Miscellany

4.1 Neutron Stars

The basic ideas developed for the surface reconstruction problem (section 2.4) have also been applied to this much more esoteric situation.

The isospin-wave modes in a neutron star were studied, taking into

account the correct expression for excitation energy and the coupling with the "soft pion modes" (ref.32,34). It was shown that the softening of isospin-wave models could lead to the formation of a proton lattice. With spin orientation such a system could have a field of 10^{15} Gauss of obvious astrophysical importance. This followed as the natural consequence of previous investigations of Anderson, Tosatti and Palmer (Nature Phys. Sci. 245, 119, 1973).

The importance of the magnetic field was emphasised (ref.33) when the electrical conductivity of the pulsar surface in the presence of a strong magnetic field was estimated. It was found that the conductivity perpendicular to the magnetic field was $\sim 10^4$ times smaller than that parallel to the magnetic field. The emissivity of the pulsar surface was found to be strongly affected by the magnetic field, and a strong polarization in the thermal radiation from the pulsar surface was predicted. If then the spectrum of the polarised thermal radiation from the pulsar surface was obtained one would have detailed information about the density, temperature and magnetic field at pulsar surface.

One other astrophysical aspect on which work was done concerns (ref. 34) the ion-ion correlation effect on Freedman's neutrino opacity. This is important in the study of supernovae. It was possible to show that in a similar way to the reduction of the X-ray scattering in liquid metals that the ion-ion effect was shown to reduce Freedman's neutrino opacity for the supernova explosion drastically. This effect was predominant for low energy neutrinos ($E \lesssim 3$ meV), and the factor of the reduction can be an order of magnitude.

Transport properties of stellar matter are important ingredients in understanding stellar evolution and stellar structure. Using theoretical techniques that have proven useful in solid state physics, Fermi liquid theory, and the theory of liquid metals we have calculated (ref. 35) the electron contribution to the electrical conductivity, the thermal conductivity, and the viscosity of neutron star matter in the absence of magnetic fields for densities less than 2×10^{14} g/cc (regions where there was solid matter). The results were also applicable to high density white dwarf matter. Variational solutions of the transport equations were used except where exact solutions exist. Transport by electrons of any energy both in the presence of a lattice and without the lattice present were considered. At temperatures very much below the Debye temperature of the lattice we were able to do only an approximate treatment of the electron-phonon interaction and for

temperatures above the melting temperatures of the lattice ionic correlations were included. Relativistic electron-electron scattering was considered, as was electron-impurity and electron-neutron scattering. This work complemented previous investigations of transport properties and extended the density regions over which we know the transport properties of dense matter.

Recent observations have shown that a number of further pulsars have "restless" behaviour of the period similar to that of the Crab and Vela pulsars which had been explained as due to "microquakes" in the crust. Also, a glitch had been observed with, possibly a new type of signature, in the pulsar PSR 1508 + 55. We suggest that these phenomena could be explained at least equally well by noisiness in the rate of creep of vorticity through the neutron superfluid in the crust, in almost precise analogy to the well-known noisy behaviour of flux creep in hard superconducting magnets. In addition, even the macroglitches, especially those in the Vela pulsar, might be caused by the catastrophic release of pinned vorticity. (ref.36.)

Nuclear Physics

In this work (ref.37) the mysterious 0^+ states of ^{16}O and ^{40}Ca explained in terms of the compressible plasma oscillations of nuclei. The theory also explained the 2^+ states which lie just above the mysterious 0^+ states. Corresponding states in other $\text{Na}(N : \text{Integer})$ nuclei were also explained. The agreement with experimentally observed states was excellent. In a similar approach a simple analytical R.P.A. model was presented to deal with the breathing modes of ^{16}O and ^{40}Ca .

A simple analytic R.P.A. model was presented to deal with the breathing modes in ^{16}O and ^{40}Ca (ref. 37). Harmonic oscillator wave functions and a Skyrme-type effective interaction was used. The eigenfunction and the eigenvalue were expressed in a very simple analytic form from ^{40}Ca . The sensitivity to the interaction however limits the quantitative usefulness of this approach as it has in others.

Finally, delving into elementary particle theory we described (ref. 38) a satisfactory strong coupling infrared limit for the asymptotically free gauge theories currently hypothesized for the strong interactions, which has many of the observed properties, including unbroken colour symmetry and absence of free quarks or gluons. In analogy with simpler problems such as the Kondo problem this was a necessary, if not sufficient, condition for scaling to go continuously from asymptotic freedom to real particles as an infrared limit.

Summary

This report we hope has given some idea of the range of work supported (albeit in most cases to a very small extent). Further details can best be found by referring to the appropriate original articles. The work of the Theory of Condensed Matter Group is of course much wider as can be seen by the appendixes lists of publications. In a sense it is this large backup which enables such a small investment on the part of the U.S.A.F. to produce such a large return.

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APPENDIXA Brief Survey of Surface Physics in Europe

Surface physics has reached large scale proportions in Europe as in the U.S.A. so in this survey we are not and indeed could not cover the whole of it. Instead we are concentrating on what we feel are important areas of work and the people within those areas who would seem to be most active and liable to achieve results. Everyone could of course complete his own list which would very probably be different from this one. For this we make no apology, the way one judges can only be subjective. We may say that the writing of this appendix has been assisted by Drs. Inglesfield, Haydock, Kinniburgh and Burt, themselves experts in the theory of surface energy, Recursion methods, LEED and photoemission. Overall the Cavendish laboratory probably contains the largest concentration of expertise on the electronic theory of surfaces anywhere in Europe. Experimental work in the Cavendish on surfaces is mainly within Professor D. Tabor's group and has, in the past, been concentrated upon mechanical properties. There has always been a small group under Dr. J. Wilson working on electron loss and Auger which is now in the process of being augmented by LEED work and expanded generally. The other surface work in the Cavendish by Dr. M. Pepper on silicon inversion layer properties is the subject of a proposal to U.S.A.F. and so will not be discussed further. The other two major institutions with large surface expertise are Dr. R.O. Jones' group at K.F.A., Institut für Festkörperforschung, Jülich, Germany and Professor S. Lundqvist's group at the Institute of Theoretical Physics, Gothenberg, Sweden. There are others of course, e.g. Max Planck Institute at Stuttgart and Nordita but we feel that these are the most active centres of surface work in Europe at the present time. In order to make this brief survey easier to read we have split it into areas of major interest. A complete list of the people and their institutions will be found at the end of this appendix.

Chemisorption, Adsorption, etc.

The search for a practical method of the calculation of the mechanics of adsorption and chemisorption continues in Europe as in America. Since the problem is so complicated it is natural that these

should split into either large scale computer calculations of idealised systems or investigations of model hamiltonians designed to either help interpret data or "bring out the physics" of the situation.

A natural starting point in any of these problems is the free surface i.e. why does a particular metal or type of surface produce a good catalyst. This is the approach of G.S. Painter, P.J. Jennings and R.O. Jones at Julich who have made a study of a cluster of atoms designed to represent smooth and stepped surfaces of iron, nickel and copper. They found that the known active stepped surface has charge lobes which stick out of the surface and may provide the sites for adsorption. Copper, which is fairly inert, does not have these. Work on this model system is continuing and we feel that it could produce some very good numerical results. An alternative numerical scheme which holds out promise is by Van der Avoird's group at M_umegen, Netherlands, where they are investigating the application of Koster Slater and L.C.A.O. calculations to the problem of semiinfinite systems and the effects of adsorption. The advantages of this over say those of the cluster calculation is that adge effects due to the finite size of the cluster are avoided. The problem with all forms of numerical methods based upon, as near as possible, ab initio assumptions is that the physics can be lost in either the numerical methods or the simplifications that have to be built in without realising it. For this reason calculations based upon model hamiltonians taking into account the major physical effects are also important if only as a check against the computer calculations. For instance Gunnarson has done some very useful work into the various extensions and limitations of the local density approximation (a universal approximation for numerical work) when used in adsorption problems. Leading exponents of these methods are Professor T.B. Grimley and his group at Liverpool and Dr. D.M. Newns and his group at Imperial College, London. Professor Grimley has been active in this area for a long time and has used a number of models for his calculations which all show a definite 'chemical' bias but he is a very strong worker in this field and has produced some excellent work in the past. Dr. Newns has been much more concerned with what might be called extreme modelling in that he simplifies the system down to its barest essentials and uses model hamiltonians (especially the Anderson). He has studied the effects of things like the image potential upon ionisation of adatoms. This type of work is

we feel, very important because, as we intimated above, much is left out of computer calculations (like the image potential) which may or may not have important effects in certain cases. In addition to this Dr. News' group has been active in the area of investigating the effect of the substrate upon photoemission from the adsorbed species. This must be understood if one is to interpret data and since it is a dynamic effect not easily calculated ab initio J. Harris of R.O. Jones' group at Julich has also performed a related calculation. This work is related directly to the experimental work of the group at Chalmers University (Sweden) in particular that of S. Andersson who uses a large array of techniques (LEED, Energy loss, etc) to study adsorbed layers on clean surfaces and is probably the best experimentalist in this field anywhere (i.e. U.S.A. included).

L.E.E.D.

Sadly most of the top people in L.E.E.D. and related techniques (e.g. RHEED) are now in the U.S.A.. For some reason it has not sustained the interest in Europe that it has in the States. The most active groups are the Groupe des Etudes Surface at Grenoble (France) including Drs. Aberdan and Bardoing, Dr. Stig Andersson at Chalmers University, Gothenberg (Sweden) and Dr. John Pendry and co-workers at the Science Research Council Laboratory at Daresbury (England). The tendency now is to use LEED as a tool in the investigation of overlayers and many of the pioneers in Europe as for instance Pendry, Forstmann (University of Bristol) and Jones have now largely moved on to new pastures. As far as applied work is concerned A.J. Van Bommel is doing nice work on overlayers in semiconductors related to practical problems of low work function emitters at Philips Research Laboratories (Netherlands) and Dr. R. Mason is applying LEED and surface chemistry ideas to transition metal surfaces, Chemistry Department, University of Sussex (England).

In the extension of the theory of LEED Dr. J. Rundgren (Stockholm University (Sweden) is doing useful work on the inclusion in LEED of the optical scattering potential to try to obtain better agreement between theory and experiment. This is a very difficult but worthwhile task. Drs Andersson and Pendry are continuing their excellent cooperation on the use of LEED which will hopefully continue even though both are now

extending their interests much more widely. But as we said before the main centres of this type of work are now to be found in the U.S.A..

Photoemission

With the advent of angular resolved photoemission techniques the rapid development of this whole area is inevitable. Because it has come into prominence in the last few years it is difficult to pinpoint a large number of European centres of excellence but we believe that, as with LEED, Dr. J.B. Pendry's group, now at Daresbury with access to the Synchrotron, will make the largest European contribution. On the experimental side Dr.R.F. Willis and co-workers at E.S.R.O. have been applying Angular resolved photoemission spectra in the study of surfaces and, using thin films, disordered systems. In Chalmers University, Gothenberg (Sweden) P.O. Nilsson and co-workers are very active in photoemission work and have applied it to a wide range of problems. They are undoubtedly the most active group in this area at this time and are producing some excellent work. On a smaller scale is the excellent work with soft X-ray appearance spectroscopy by Dr. C. Webb and Dr. P. Williams who are at present at Imperial College, London. Mention has already been made in the section on Chemisorption of the work of Newns and Harris.

In general we would say that this is an expanding field with an excellent chance of producing very great returns. The groups to watch in Europe are undoubtedly the ones at Daresbury and Gothenberg.

General Surface Theory

Despite the advances in recent years the general theory of surface properties, be they single particle (surface states etc) or collective phenomena (plasmons) are still very active fields in Europe.

If we start from the single particle properties of surfaces then we must immediately conclude that as far as the simple metals and semiconductors are concerned the major work is at present being performed in the U.S.A.. In particular we have no group willing to compete with either Appelbaur and Hamman of Bell Labs. or Marvin Cohen et.al. of Berkeley. The main emphasis in Europe is now on the transition metals and to some extent is motivated by possible chemisorption application. Apart from our own group at

Cambridge (Dr. Haydock and Professor Heine) who have applied their resolvent techniques to transition metal surfaces the main work on surface states is being performed by Dr. F. Cyrot-Lackmann and co-workers who have investigated thoroughly, using tight binding techniques, surface densities of states and their applications to general surface properties. The presence in this group of Dr. M.C. Desjonqueres and C. Hodges gives it a very strong basis for further excellent work, (Institut Laue Langevin, Grenoble, France). The cluster calculations, mentioned earlier, by the Julich group could equally be applied to these problems though the emphasis there will probably go towards small molecules rather than true surfaces.

A major problem in surface physics has always been to what extent the surface considered really related to the expected two dimensional projection of the bulk lattice. Deviations from a true surface are in most cases small taking the form of either a superlattice or a relaxation of the outermost atoms towards the bulk (or both). This is an important problem since it opens up the possibility of spin density waves or excitonic insulators and in Europe the expert is undoubtedly Dr. E. Tosatti (Istituto di Fisica, University de Roma, Italy). Of course the theory of these soft modes, charge density waves etc. is all connected with layer materials and superconductivity but on surfaces we are at least now getting to grips with the problem of calculating these effects.

Surface reconstruction is to some extent a collective phenomena and undoubtedly the major effort in Europe has been, and still is, towards an understanding of such basic properties as surface energy and role of plasmons. In this problem the major European workers J. Harris and R.O. Jones, (Julich), J. Inglesfield (Cambridge) and E. Wikborg (Gothenberg), J.C. Inkson (Cambridge) and C. Hodges (Grenoble) have taken a different viewpoint from the numerical work of N. Lang and W. Kohn in the states. They have concentrated upon the dielectric response of the surface and calculated the various properties from this. The results of these efforts have been a much greater understanding of the role of the surface plasmons in surface properties though one must be frank and admit that to some extent the argument is a pedagogical one since the total results in the calculations are fairly invariant and only the contributions from the various processes vary between authors. Much of this work is now a few years old and so has no place

in this appendix but Inglesfield and Wikborg remain active in this area and are now concerned with Van der Waals interactions between metals and using the experience gained at surfaces to help produce a more consistent many body potential for use in more general small systems (e.g. molecules, etc). J. Harris and R.O. Jones are of course now more concerned with chemisorption related properties but they have still an interest in this area. J. Harris in particular has worked recently upon the Van der Waals interaction and also extensions of the classical image potential.

Finally in this area of general surface theory there is the problem of the interaction of the collective modes with incoming electrons. This gives rise to both the image potential and also, if the electron has a high enough energy, to the creation of surface plasmons and subsequent finite lifetime of the electron. This has been studied by a number of people, in particular by D.M. Newns at Imperial College, London, J. Heinrich at Liege, Belgium and P. Echenique, R.H. Ritchie and J.C. Inkson in Cambridge. It is an important problem since there are a number of experimental possibilities which could be analysed if a reasonable theory could be worked out. Our own feeling at this time is that the semiclassical treatments of Newns and Heinrichs have serious limitations in what is essentially a quantum problem so that a method based upon our own self energy formulation would be necessary. But work is continuing along these lines at all the above places.

Conclusions

Surface physics is still very active in Europe in most cases it is at least as good as the best in the U.S.A., though there is often a different emphasis. In some cases however we are sadly lacking in part due to a limitation of computer facilities which make large scale numerical calculations the prerogative of a very few centres, though limited communication and cooperation may have something to do with it.

The major centres of surface expertise are undoubtedly at Gothenberg, Julich and Cambridge though the Grenoble complex must also be considered in any discussion of transition metals and their properties. We feel that in general surface work in Europe is of high standard and will continue to expand rapidly in the next few

years with photoemission and the treatment of real, i.e. non jellium surfaces, producing the major results. We can not see progress in chemisorption being so rapid, it is a problem of quite a different magnitude.

Surface Workers and Groups mentioned in this Appendix

Where there are a large number of co-workers only the senior man has been listed.

1. Chalmers University, Gothenberg, Sweden.
 - S. Lundqvist (Many body theory)
 - S. Andersson (Chemisorption, LEED, photoemission, etc.)
 - A P.O. Nilsson (Photoemission)
 - I.O. Gunnarsson (Chemisorption, bandstructure theoretician)
 - E. Wikborg (Many body theory of surfaces).
2. Institut fur Festkorperforschung, K.F.A. Julich, Germany.
 - R.O. Jones (Head of group, theoretician on general surface problems)
 - J. Harris (Theoretician).
3. E.S.R.O., Noordwyk, Netherlands.
 - R.F. Willis (Photoemission etc., experimentalist).
4. University of Nijmegen, Netherlands.
 - A. Van der Avoird (LCAO etc calculations and their application to chemisorption).
5. Philips Research Laboratory, Eindhoven, Netherlands.
 - A.J. Van Bommel (LEED, experimentalist studying overlayers)
 - H.H. Brongersman (Ion scattering from surfaces, experimentalist).
6. Institut Laue Langevin, Grenoble, France.
 - F. Cyrot-Lackmann (Theoretician, wide interests in transition metals)
 - M.C. Desjonqueres (Theoretician, surfaces in general, many body theory).
7. Istituto di Fisica, Universita di Roma, Italy.
 - E. Tosatti (Theoretician, wide interests, semiconductors, surfaces).

8. University of Liverpool, Liverpool, England.
T.B. Grimley (Extensive interests in chemisorption and surfaces).
9. Imperial College, London, England.
D.M. Newns (Theoretician extensive interest in surfaces
chemisorption plasmons etc.)
C. Webb }
P. Williams } (Experimentalists, soft X-ray appearance
 } spectroscopy).
10. Science Research Council Laboratory, Daresbury, Warrington, England.
J.B. Pendry (Theoretician, LEED, RHEED, photoemission etc).
11. Cavendish Laboratory, Madingley Road, Cambridge, England.
V. Heine, J.C. Inkson and Theory of Condensed Matter
Group - see main report.